

Numerical modeling of unsaturated porous media as a two and three phase medium: A comparison

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ABSTRACT: A numerical simulation of the hydro-mechanical behaviour of an unsaturated porous medium is presented. The coupled hydro-mechanical model used is based on the continuum theory of mixtures and treats the unsaturated soil as a three phase porous medium (solid, liquid and gas). Principal variables are the solid deformation, the liquid pressure and the gas pressure. The two fluid phases are in motion and a non-linear pore pressure - saturation relation is used. The resulting system of equations is discretized in space using the finite element technique and in time by the Θ - method. The comparison of numerical results and experimental test data shows that this hydro-mechanical model is capable to reproduce the principal phenomenon in the case of a hydric solicitation. The three phase formulation is compared to a simplified version considering only a two phase medium with static air phase. Merits and shortcomings of the two approaches are shown.

1. HYDRO-MECHANICAL MODEL

1.1 Introduction

The hydro-mechanical behavior of unsaturated soils can be modeled via a formulation based on the momentum and mass balance equations of its three phases: solid, liquid (water) and gas (air). If one allows for interaction between the phases, flow of the fluids and skeleton deformation (in the following linear elastic), the numerical model achieved covers most of the important features of unsaturated soils.

In this paper, we use the definition of unsaturated soil as a mixture of three phases: solid, water and air. However, according to the mixture theory, such a mixture would be saturated in the sense that the three phases occupy the full volume (no empty space).

In the following, we will report the main equations that can be found using an approach based on work by Hassanizadeh & Gray (1979) and Schrefler *et al.* (1990). For details of the derivation the reader is referred to Klubertanz *et al.* (1997)

1.2 Balance equations

The momentum balance of the three phase mixture, reads

$$\nabla \bullet (\sigma'_{ij} - S^w p^w \delta_{ij} - (1-S^w) p^a \delta_{ij}) + \rho g_i = 0 \quad (1)$$

where σ'_{ij} is the effective stress tensor, p^w and p^a the water and the air pressure, g_i the gravity vector and ρ the density of the mixture as $\rho = (1-n) \rho^s + n S^w \rho^w + n S^a \rho^a$. Note that here ρ^s , ρ^w and ρ^a are the solid, water and air true densities respectively. S^w is the water saturation, defined as the ratio of water volume divided by the total pore volume and S^a the degree of air saturation, defined as the ratio of air volume divided by the total pore volume. Further n denotes the porosity, δ_{ij} the Kronecker delta and $\nabla \bullet$ the divergence operator. Please note that throughout this paper quantities related to the solid, water or air phase are denoted by the superscripts s , w and a respectively.

The mass balance equations read (Klubertanz *et al.*, 1997)

$$\left(\frac{n}{S^w} \frac{\partial S^w}{\partial p^c} + \frac{n}{\rho^w} \frac{\partial \rho^w}{\partial p^w} \right) \frac{\partial p^w}{\partial t} - \frac{n}{S^w} \frac{\partial S^w}{\partial p^c} \frac{\partial p^a}{\partial t} + \nabla \bullet v^s + \nabla \bullet v^{ws} + v^w \nabla n + \frac{n}{S^w} v^w \nabla S^w + \frac{n}{\rho^w} v^w \nabla \rho^w - \frac{1}{\rho^s} v^s \nabla n = 0 \quad (2)$$

for the summed water - solid balance and

$$\left(\frac{n}{1-S^w} \frac{\partial S^w}{\partial p^c} + \frac{n}{\rho^a} \frac{\partial \rho^a}{\partial p^a} \right) \frac{\partial p^a}{\partial t} - \frac{n}{1-S^w} \frac{\partial S^w}{\partial p^c} \frac{\partial p^w}{\partial t} + \nabla \bullet v^s + \nabla \bullet v^{as} + v^a \nabla n - \frac{n}{1-S^w} v^a \nabla S^w + \frac{n}{\rho^a} v^a \nabla \rho^a - \frac{1}{\rho^s} v^s \nabla n = 0 \quad (3)$$

for the summed air - solid balance, both for incompressible grains.

In (2) and (3) v^π means the Lagrangian velocity of the π -th phase ($\pi = s, w, a$).

Note in passing that for the derivation of (2) and (3) $S^a = 1-S^w$ and that $v^{\pi s} = n(v^\pi - v^s)$ is used. Additionally, it is assumed that the degree of water saturation S^w is only a function of the capillary pressure defined as $p^c = p^w - p^a$ (see below), as well as ρ^π being a function of the pressure p^π exclusively (except for the grain, where ρ^s is constant).

1.3 Simplified mass balances

The solid is assumed to be linear elastic and the air phase governed by the ideal gas law; furthermore, the relative fluid - solid velocity is governed by Darcy's law (Gray & Hassanizadeh, 1991).

Under those assumptions and neglecting higher order terms one finally finds

$$\left(\frac{n}{S^w} \frac{\partial S^w}{\partial p^c} + \frac{n}{\rho^w} \frac{\partial \rho^w}{\partial p^w} \right) \frac{\partial p^w}{\partial t} - \frac{n}{S^w} \frac{\partial S^w}{\partial p^c} \frac{\partial p^a}{\partial t} + \nabla \bullet v^s + \nabla \bullet \left(\frac{k_{rw} K}{\mu^w} (\nabla p^w - \rho^w \mathbf{g}) \right) = 0 \quad (4)$$

for the water - solid balance and

$$\left(\frac{n}{1-S^w} \frac{\partial S^w}{\partial p^c} + \frac{n}{\rho^a} \frac{\partial \rho^a}{\partial p^a} \right) \frac{\partial p^a}{\partial t} - \frac{n}{1-S^w} \frac{\partial S^w}{\partial p^c} \frac{\partial p^w}{\partial t} + \nabla \bullet v^s + \nabla \bullet \left(\frac{k_{ra} K}{\mu^a} (\nabla p^a - \rho^a \mathbf{g}) \right) = 0 \quad (5)$$

for the air - solid balance.

The relative permeability k_{rw} of water is supposed to be a function of the degree of saturation and of the porosity (Seker, 1983), the relative permeability of air k_{ra} being a function of the porosity only. K is the geometric permeability.

A capillary pressure - saturation relation reported by Seker (1983) which has been obtained by tests on different materials has been used:

$$S^w = \frac{1}{\left(\frac{1}{\Psi_0} \log \left(-\frac{c_d p^c}{g_z \rho^w} \right) \right)^{\frac{1}{\Psi_1}} + 1} \quad (6)$$

where Ψ_0 , Ψ_1 and c_d are material parameters and g_z represents the vertical component of the gravity vector.

Equations (1), (4) and (5) represent a set of three equations for the three unknowns solid displacement, u_i , air pressure p^a and water pressure p^w (u_i being, of course, linked to σ'_{ij} in (1) via a constitutive equation, in this case linear elastic, and to v^s via derivation in time). Other choices for the set of unknowns are of course possible.

1.4 Two phase model

A more commonly used formulation consists in a two phase model with so called static air phase. This corresponds to an unsaturated mixture in the sense of the mixture theory, i.e. the pore volume is partly empty. Assuming constant air pressure $p^a = p^{\text{atmospheric}}$ and setting this reference pressure $p^{\text{atmospheric}} \equiv 0$, one can easily derive such a model from (1) and (4), yielding

$$\nabla \bullet (\sigma'_{ij} - S^w p^w \delta_{ij}) + \rho g_i = 0 \quad (7)$$

for the momentum balance and

$$\left(\frac{n}{S^w} \frac{\partial S^w}{\partial p^c} + \frac{n}{\rho^w} \frac{\partial \rho^w}{\partial p^w} \right) \frac{\partial p^w}{\partial t} + \nabla \bullet v^s + \nabla \bullet v^{ws} = 0 \quad (8)$$

for the solid - water mass balance. The remaining system is of two equations for the two unknowns u_i and p^w .

2. DISCRETIZED SYSTEM

Using a standard Galerkin procedure and the Θ -Method for discretisation (e.g Zienkiewicz, 1977), one finds the following system of equations for the three phase model, equations (1),(4),(5)

$$\mathbf{K} \mathbf{u}_{n+1} + \mathbf{L}^w p_{n+1}^w + \mathbf{L}^a p_{n+1}^a = \mathbf{F}_{n+1}$$

$$\mathbf{L}^{wT} \mathbf{u}_{n+1} + (\mathbf{M}^w + \Delta t \Theta \mathbf{H}^w) p_{n+1}^w + \mathbf{N}^{wa} p_{n+1}^a = \mathbf{L}^{wT} \mathbf{u}_n + (\mathbf{M}^w - (1-\Theta) \Delta t \mathbf{H}^w) p_n^w + \mathbf{N}^{wa} p_n^a + \Delta F_{n+1}^w$$

$$\mathbf{L}^{aT} \mathbf{u}_{n+1} + (\mathbf{M}^a + \Delta t \Theta \mathbf{H}^a) p_{n+1}^a + \mathbf{N}^{aw} p_{n+1}^w = \mathbf{L}^{aT} \mathbf{u}_n + (\mathbf{M}^a - (1-\Theta) \Delta t \mathbf{H}^a) p_n^a + \mathbf{N}^{aw} p_n^w + \Delta F_{n+1}^a \quad (9 \text{ a-c})$$

In (9 a-c) \mathbf{K} is the rigidity matrix, \mathbf{L}^w and \mathbf{L}^a the liquid and gas flow matrices receptively and \mathbf{F}^a the loading vectors. The other matrices are given in the appendix.

For the case of the two phase model, the discretized system (9) would consist in equations (9 a,b) without the p^a - terms.

3. EXPERIMENT

The case studied is the drainage of a sand column. It can be considered representative for a wide range of gravity - governed unsaturated soil behaviour since no external loads are applied and the deformation and desaturation depends only on the soil and fluid parameters. Coupling between the phases is expected to be crucial.

The corresponding laboratory experiments have been carried out by Liakopoulos (1964). In these tests water is allowed to flow through a sand

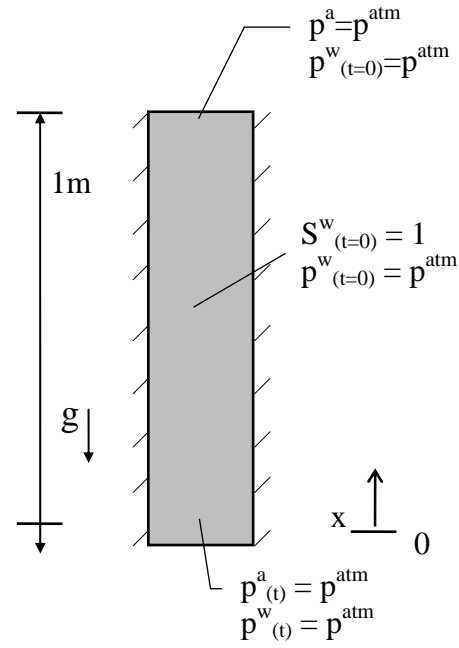


Figure 1: Initial and boundary conditions

Parameter	Value
Young's modulus	$E=1.3 \cdot 10^6 \text{ Pa}$
Poisson's ratio	$\nu=0.4$
porosity	$n=0.297$
gravity acceleration	$g=9.81 \text{ m/s}^2$
water viscosity	$\mu^w=10^{-3} \text{ Pas}$
air viscosity	$\mu^a=1.8 \cdot 10^{-5} \text{ Pas}$
solid (grain) density	$\rho^s=2700 \text{ kg/m}^3$
water density	$\rho^w=1000 \text{ kg/m}^3$
air density	$\rho^a=1 \text{ kg/m}^3$
intrinsic permeability	$K=4.5 \cdot 10^{-13} \text{ m}^2$

Table 1: Material parameters
(see also Gawin *et al.*, 1996)

column. The measurement starts when the water disappears from the surface. Both upper and lower end of the column are exposed to atmospheric pressure. The side walls are rigid and impermeable for both water and air. The initial conditions are consequently $S^w=1$ and $p^w=p^{\text{atm}}$ ($=0$) all over the column (see also Fig.1). Material parameters are given in Table 1.

Measurements of pressure at several points of the column and outflow at the bottom are available as discrete functions of time. Liakopoulos (1964) measured pore pressure and water outflow during desaturation.

4. NUMERICAL SIMULATION

The above models are applied to Liakopoulos (1964) experiment introduced in the previous chapter. Material parameters in Table 1 are used. With $\Psi_0=3.1$, $\Psi_1=0.18$ and the dimensional constant $c_d=100 \text{ m}^{-1}$ in (6) the capillary pressure - saturation data given by Liakopoulos is reproduced reasonably well. The residual degree of air saturation is set to $S_r^a = 1\%$. All results are calculated for a reference pressure of $p_0 = 0$.

4.1 Comparison with experiments

In Figure 2 the calculated results of the three phase model for the pore pressure vs. column height for several time steps (solid lines) are given and compared with the experimental data (dotted lines with symbols).

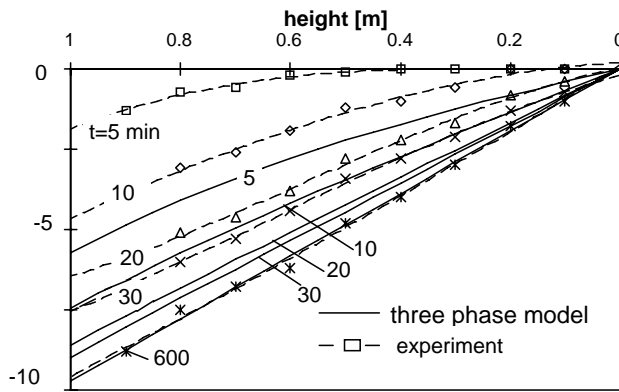


Figure 2: Pore pressure vs. column height; experimental results (dotted lines with symbols) and three phase calculation (solid lines)

Already after 20 minutes there is a good agreement between computations and measurements, even if discrepancies in the early part can be seen. Those may partly be due to the simplifications during the derivation of equations (4) and (5) (for a detailed discussion, see Klubertanz *et al.*, 1997). Another possible source of error is the employed capillary pressure - saturation relation (6). Figure 3 shows the computed outflow at the lower end of the column compared with experimental data. The calculated results match the experimental data very well.

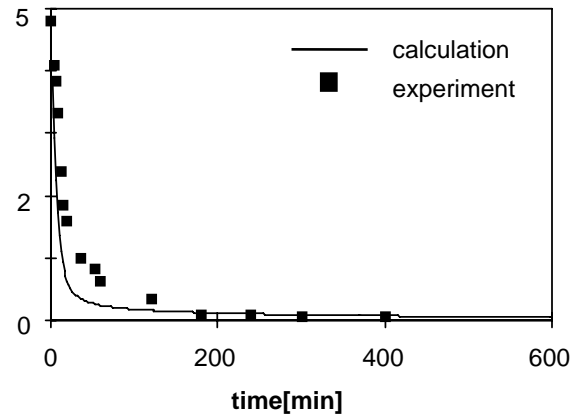


Figure 3: Water outflow vs. time

4.2 Two and three phase calculation

Figures 4 to 8 show comparisons between the two phase model with static air phase (i.e. $p^a(t) = \text{const.} = p^{\text{atmospheric}}$, Equations (7),(8)) and the full three phase model ((1),(4),(5)).

In the three phase case equilibrium is reached much faster than the two phase case (see Figures 4 and 5). One can see that in the early stages of the experiment, the two phase model matches the experimental results better than the three phase model (cf. Fig. 5 and 2).

Figure 6 represents the air pressure for selected time steps over the column heights. It can be seen that this pressure reaches important values and is of the same order of magnitude as the porewater pressure. This is important for the suction $p^c = p^w - p^a$ (see Figure 7), which shows significant differences compared with the two phase case, as would have been expected.

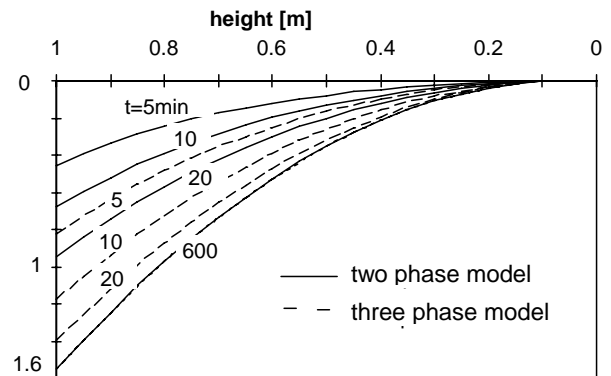


Figure 4: Displacement for two (solid lines) and three (dotted lines) phase calculations (results for $t = 600\text{s}$ are identical)

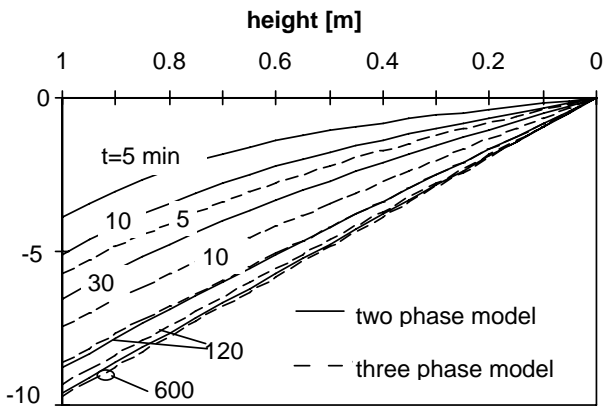


Figure 5: Water pressure for two (solid lines) and three (dotted lines) phase calculations

The consequences on the degree of saturation, which is, for the chosen relation (6), a nearly linear function of the suction in the range of interest, are important, as can be seen in Figure 8. Note that the maximum degree of saturation is only 99%, which is due to computational stability reasons. Other ways of stabilizing the solution for degrees of saturation near 100% are possible and lead to comparable results.

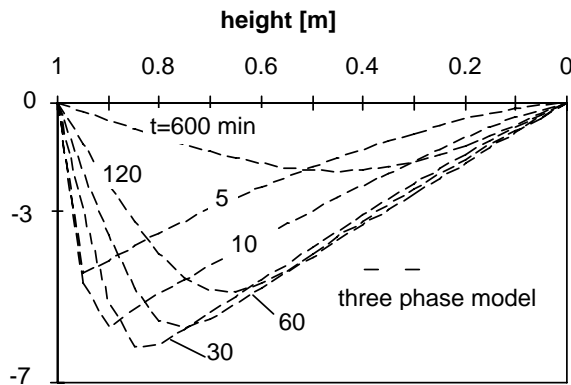


Figure 6: Air pressure for three phase calculations

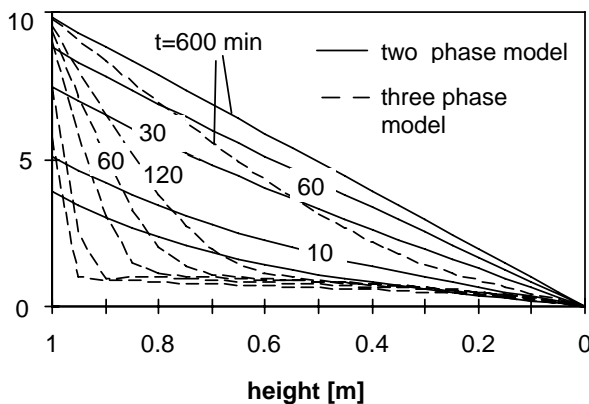


Figure 7: Suction for two (solid lines) and three (dotted lines) phase calculations

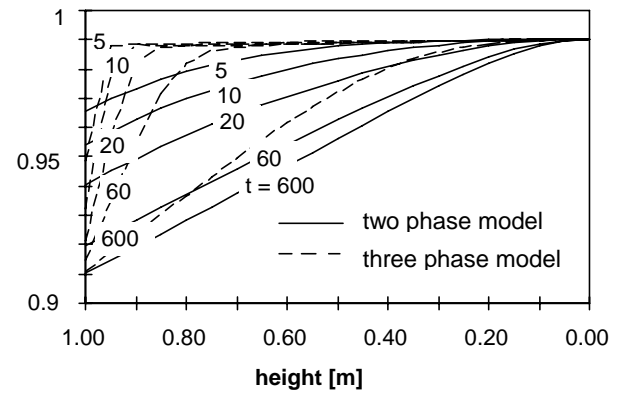


Figure 8: Degree of saturation for two (solid lines) and three (dotted lines) phase calculations

In the above figures differences between two and three phase calculations are significant and underline, at least for this particular case, the importance of a fully coupled three phase approach to model unsaturated soils. With only two phases, the calculation seems to miss characteristic features of the unsaturated soil behavior which in certain applications may become important, especially for the prediction of the evolution of S^w .

As far as the early part of the experiment is concerned, the two phase model seems to work better. Physically the soil is almost fully saturated at the beginning (degree of saturation near $S^w=1$) and the air phase is discontinuous, violating the assumption in the three phase model. For such a particular situation, the two phase model is consequently more appropriate.

5.CONCLUSION

It has been shown that the proposed models reproduce relatively well most of the experimental results (pore water pressure and outflow). In the early part of the transient process the two phase model shows better results. It can be seen that the differences between a two and a three phase model are important and that it is necessary to consider a fully coupled three phase calculations in order to correctly simulate unsaturated soil behavior, namely to compute the degree of saturation. The model can be extended to two or three dimensional problems and to include elasto-plastic solid behavior.

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APPENDIX

The matrices in equation (9 a-c) read in detail, using standart notation (Zienkiewicz, 1977):

$$M^w = \int_{\Omega} n \left(\frac{\partial \mathcal{S}^w}{\partial p^c} + \frac{S^w}{\rho^w} \frac{\partial \rho^w}{\partial p^w} \right) N^T N d\Omega$$

$$H^w = \int_{\Omega} S^w K^w \nabla N^T \nabla N d\Omega$$

$$N^{wa} = \int_{\Omega} n \frac{\partial \mathcal{S}^w}{\partial p^c} N^T N d\Omega$$

$$M^a = \int_{\Omega} n \left(\frac{\partial \mathcal{S}^w}{\partial p^c} + \frac{1-S^w}{\rho^a} \frac{\partial \rho^a}{\partial p^a} \right) N^T N d\Omega$$

$$H^a = \int_{\Omega} (1-S^w) K^a \nabla N^T \nabla N d\Omega$$

$$N^{aw} = \int_{\Omega} n \frac{\partial \mathcal{S}^w}{\partial p^c} N^T N d\Omega$$